Mechanical anisotropy of energetic polycrystals as possible initiation mechanism

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Abstract. The dislocation model is used to estimate the plastic strain in high explosive (HE) crystals at relatively low impact velocities. Due to anisotropic distribution in orientation of HE grains the localization of heat production is observed. At certain impact velocities this heating is sufficient to induce chemical reactions with energy release.

1. Introduction

Safety of different devices, which contain high explosives (HE) such as octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX), is determined largely by chemical reactions initiated by impact on HE with different velocities. The impact loading may lead to high pressure (more than 10 GPa) or to low pressure (less than 1 GPa). Many phenomenological models were developed for high-pressure impacts [1, 2]. These models are widely used for HE reactions predictions in engineering. But the commonly accepted models for low-pressure impacts are lacking. This fact is connected with complex and multiscale processes involved in the phenomena in question. The complexity of determination of the leading process stems from many reasons for generation of detonation centers such as HE heterogeneity, HE deformation process instability, and friction of material grains.

Here we consider localization of heat production by means of plastical deformation due to anisotropic orientation distribution as leading process of chemical reactions beginning.

2. Dislocation model for plastic strain in a single crystal

The elasto-plastic deformation of material grains conglomerate is known to be sufficiently anisotropic, and thus its behavior depends on loading direction. The anisotropic mechanical properties of the material is defined by its bulk anisotropic elastic characteristics and various plasticity deformation mechanisms (dislocations, twins and martensite transformations) for different spatial orientations of material grains. Complicated picture of elasto-plastic deformation is formed on account of anisotropic properties of material grains and its interaction.

The system of equations for single HE crystal with accounting for dislocation motion in

Lagrangian coordinates for 1D case [3–5] is

$$\frac{1}{\rho}\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\frac{\partial u}{\partial x}, \tag{1}$$

$$\rho\frac{\mathrm{d}u}{\mathrm{d}t} = \frac{\partial \sigma_{xx}}{\partial x}, \tag{2}$$

$$\rho\frac{\mathrm{d}E}{\mathrm{d}t} = -\frac{\sigma_{xx}}{\rho}\frac{\mathrm{d}\rho}{\mathrm{d}t} + \frac{\partial}{\partial x}\left(K\frac{\partial T}{\partial x}\right), \tag{3}$$

$$\sigma_{xx} = -P(\rho, E) + S_{xx}, \tag{4}$$

$$\frac{\mathrm{d}S_{xx}}{\mathrm{d}t} = \frac{4}{3}G\frac{\partial u}{\partial x} - 2G\frac{\mathrm{d}w_{xx}^{\mathrm{pl}}}{\mathrm{d}t}, \tag{5}$$

$$\frac{\mathrm{d}w_{xx}^{\mathrm{pl}}}{\mathrm{d}t} = -\frac{1}{\sqrt{6}}Vb\rho_D, \tag{6}$$

$$\frac{m_0}{(1 - V^2/c_t^2)^{3/2}}\frac{\mathrm{d}V}{\mathrm{d}t} = -\frac{3}{4}b\left(\sqrt{\frac{2}{3}}S_{xx} \pm \frac{2}{3}Y\right) - B(V,T)V, \tag{7}$$

where ρ is the density, u is the mass velocity, σ_{xx} is the stress tensor, S_{xx} is the stress tensor deviator, P is the pressure, V is the dislocation velocity, ρ_D is the dislocation density, Y is the yield stress, G is the shear modulus. For dislocation density evolution equation [4]

$$\frac{\mathrm{d}\rho_D}{\mathrm{d}t} + \rho_D\frac{\partial u_k}{\partial x_k} = \left(\delta_0\frac{Y_0}{Gb} + \delta_f\sqrt{\rho_D} - k_a b\rho_D\right)|V|\rho_D \tag{8}$$

is used. Yield stress is determined using the Taylor relation [6]:

$$Y = Y_0 + \alpha Gb\sqrt{\rho_D}. \tag{9}$$

Parameters for the dislocation motion are taken from [5], where the phonon drag coefficient is calculated via the molecular dynamics.

The system of equations described above is written for the case of loading direction along the [001] direction. The elasto-plastic deformation of a material grains conglomerate is known to be sufficiently anisotropic. So we need to extend this model for any loading direction. For this reason the angles between loading direction and [001] direction are set in each grain. Then the stress and the strain tensor are transformed from laboratory to local coordinate system, which relates to the [001] direction. For simplicity, we consider 2D case of orientation distribution of crystals, where the orientation axes are varied in xy–plane (θ is the material orientation angle):

$$\sigma_L = q^T\sigma q, \tag{10}$$

$$\varepsilon_L = q^T\varepsilon q. \tag{11}$$

The orthogonal transformation matrix is given by

$$q = \begin{pmatrix} \cos(\theta) & -\sin(\theta) & 0 \\ -\sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{12}$$

After calculation, the stress is transformed back to the laboratory system:

$$\sigma = q\sigma_L q^T. \tag{13}$$

This dislocation deformation model was implemented in CSPH-VD3 code [8]. This code is developed at VNIIA and based on contact smoothed particle hydrodynamics method [9]. The software was tested on flying plate experiment [7] for aluminium. In this experiment aluminium impactor with velocity 660 m/s and 0.4 mm thickness strikes at aluminium target with 2.93 mm thickness. Free surface velocity time dependence was measured. Single aluminium crystal was

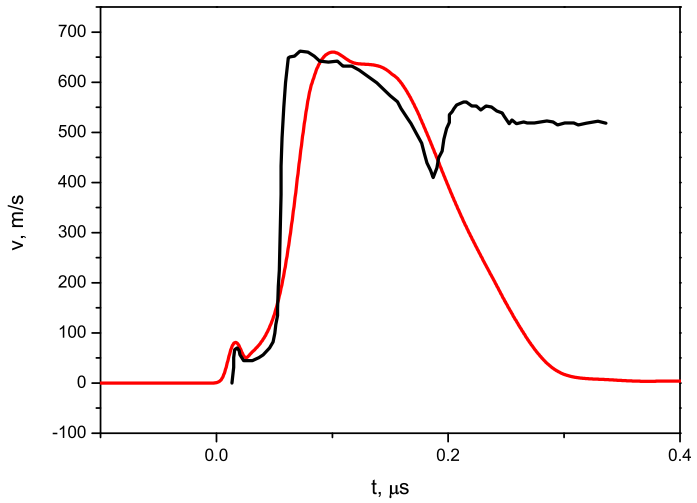

Figure 1. Free surface velocity of aluminium target at temperature 688 K. Simulated data is shown by the red line, black line is the experimental data [7]. Material fracture is not considered at simulation.

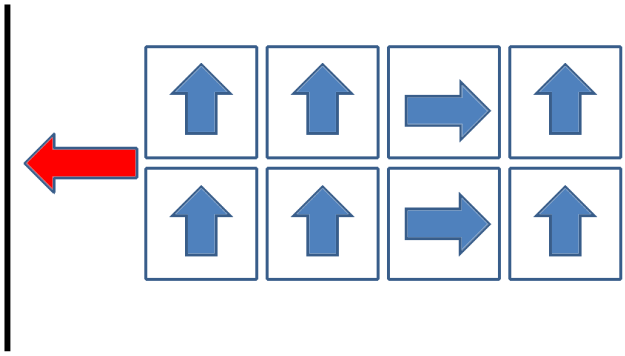

Figure 2. Schematic view of 16 HE crystals system are shown (side view). System motion is shown by the red arrow. Dislocation motion in each grain is shown by blue arrows.

simulated with impact direction alongside material orientation direction [001]. Parameters for aluminium dislocation model are taken from [5]. Experimental and simulated data comparison is illustrated in figure 1. It is seen from this figure that shock wave thickness for calculated results is larger than experimental. This fact is due to temperature non linearity of model parameters such as phonon drag, dislocation multiplication and annihilation coefficients.

3. Strain localization for HE

Consider the shock wave loading of HE crystals system with the strong anisotropy in mechanical properties (figure 2). 16 grain complex are chosen. 4 grains of it have [001] material orientation along impact direction. Remain grains orientations are chosen for dislocation motion perpendicularly for impact direction, so plastical deformation are almost inhibited here. Each grain is a cube with 50 micrometers leg. Dislocation deformation model from the previous section is set for each grain. Available model parameters for anisotropic elastic modulus for HMX are taken from [10]. We assume, due to the lack of data, that all the plastic work is converted to heat. For burn rate the Arrhenius-type relation is applied:

$$\frac{\mathrm{d}\lambda}{\mathrm{d}t} = Z(1-\lambda)\exp\left(-\frac{E_a}{RT}\right), \tag{14}$$

where T is temperature, Z is kinetic rate constant, E is activation energy per mole, R is the universal gas constant, λ is burn rate ($\lambda = 0$ means no reaction, $\lambda = 1$ corresponds to fully burned). These parameters for HMX are taken from [11].

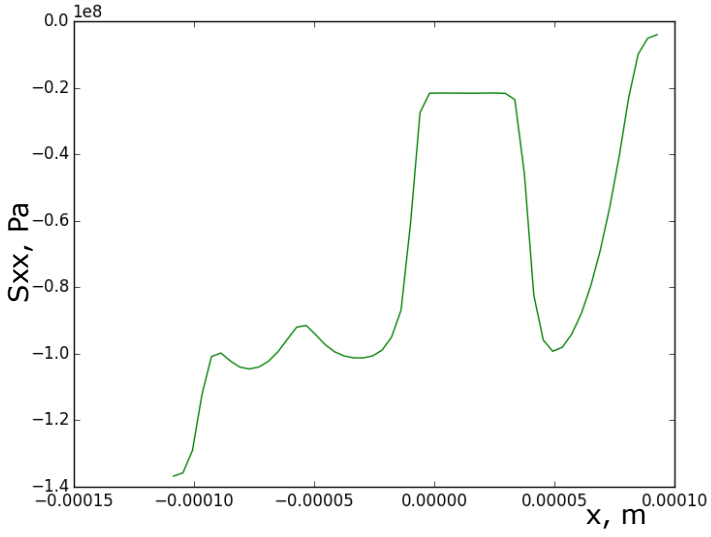

Figure 3. Stress deviator profile (Pa) at time 6.06×10^{-8} s. Impact velocity is 200 m/s.

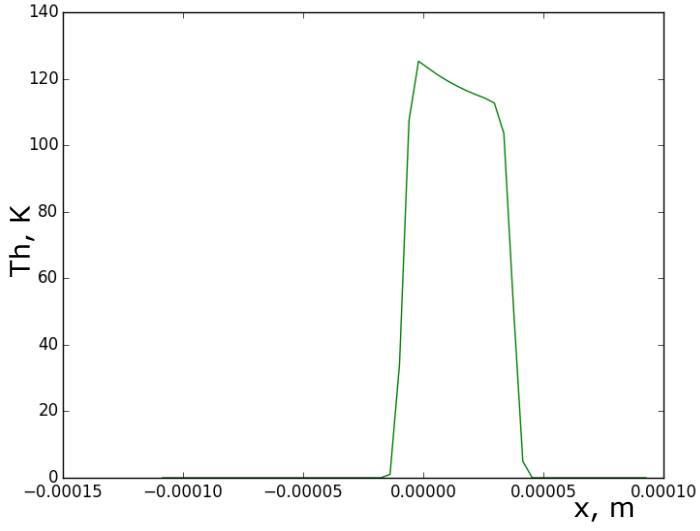

Figure 4. Temperature of heating profile (K) at time 6.06×10^{-8} s. Impact velocity is 200 m/s.

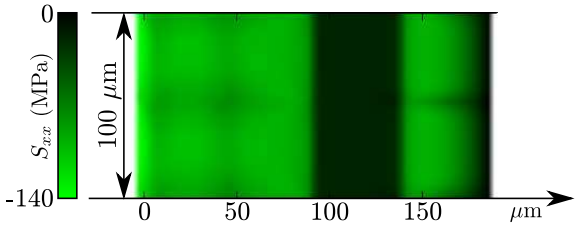

Figure 5. Stress deviator contour at time 6.06×10^{-8} s. Impact velocity is 200 m/s.

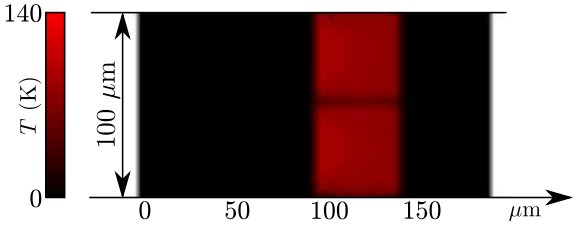

Figure 6. Temperature of heating contour at time 6.06×10^{-8} s. Impact velocity is 200 m/s.

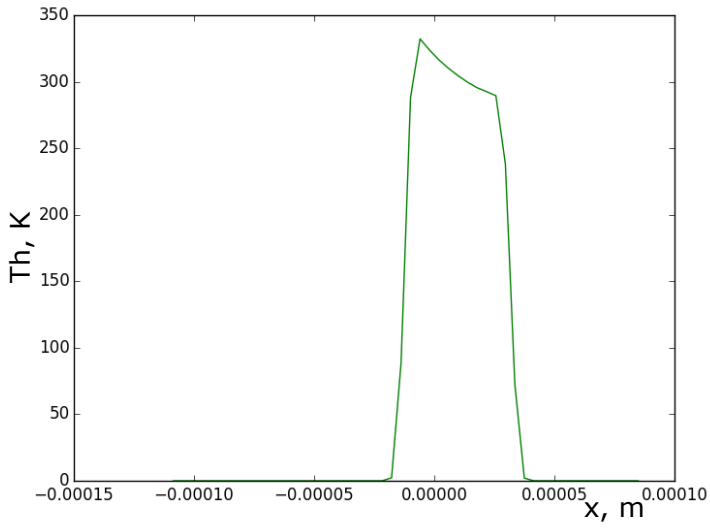

Figure 7. Temperature of heating profile (K) at time 6.52×10^{-8} s. Impact velocity is 350 m/s.

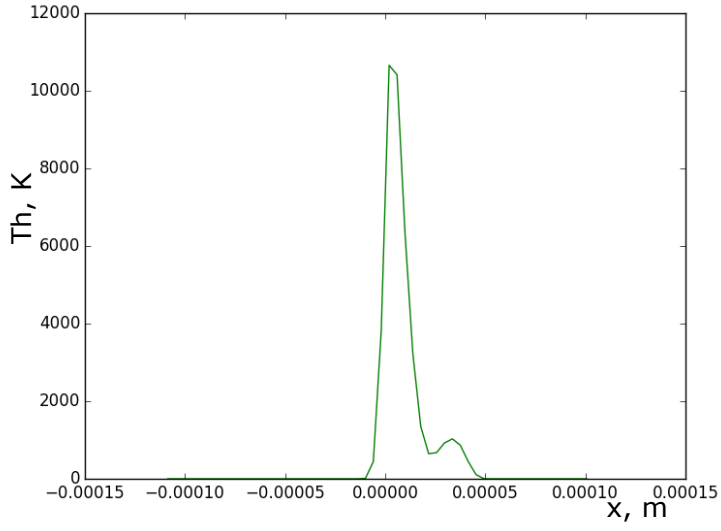

Figure 8. Temperature of heating profile (K) at time 1.05×10^{-7} s. Impact velocity is 350 m/s.

This system impacts the rigid wall at the velocity of 200 m/s. The results of the simulation are shown in figures 3–6. At this impact velocity the heating temperature is about 120 K. The burn fraction is very low (about 10^{-16}). Let us increase the impact velocity up to 350 m/s. The temperature of heating due to mechanical energy dissipation is shown in figure 7. This temperature is sufficient for HE chemical reaction initiation (figure 8) with the energy release.

4. Conclusion

We demonstrated that the process of HE explosive transformation can be initiated by the localization of plastic work due to the mechanical anisotropy of HE crystals.

Acknowledgments

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